

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX091622\
 Data File : VX031419.D
 Acq On : 16 Sep 2022 18:46
 Operator : JC/MD
 Sample : N4645-01
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 TOLL-MW-02

Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X091422W.M
 Title : SW846 8260

Signal : TIC: VX031419.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.252	23	27	28	rBV	10897	14475	2.03%	0.411%
2	1.593	74	83	91	rVB6	9143	29380	4.12%	0.835%
3	1.746	102	108	113	rBV	14159	19905	2.79%	0.566%
4	2.782	270	278	280	rBV2	8179	15263	2.14%	0.434%
5	2.825	280	285	300	rVV	21754	50251	7.04%	1.428%
6	3.105	322	331	342	rBV2	38416	89831	12.58%	2.553%
7	4.300	518	527	541	rVB2	39886	115572	16.19%	3.284%
8	5.391	694	706	714	rBV	84702	246179	34.48%	6.995%
9	5.477	714	720	725	rVV2	20038	56134	7.86%	1.595%
10	5.556	725	733	750	rVB	85451	246432	34.52%	7.002%
11	5.836	770	779	789	rVB7	2345	7337	1.03%	0.208%
12	5.958	789	799	809	rBV	94389	245842	34.43%	6.986%
13	6.257	838	848	857	rVB3	4057	11857	1.66%	0.337%
14	6.367	857	866	874	rBV5	3112	7932	1.11%	0.225%
15	6.763	922	931	944	rBV	133195	316205	44.29%	8.985%
16	7.098	976	986	994	rBV3	10795	26748	3.75%	0.760%
17	7.379	1018	1032	1039	rBV4	7954	18134	2.54%	0.515%
18	7.489	1044	1050	1058	rBV3	5408	12011	1.68%	0.341%
19	8.598	1226	1232	1235	rBV	7977	13725	1.92%	0.390%
20	8.653	1235	1241	1249	rVB	450235	713932	100.00%	20.286%
21	8.976	1287	1294	1299	rVB5	9042	18355	2.57%	0.522%
22	9.561	1386	1390	1395	rVB	6232	8881	1.24%	0.252%
23	10.055	1465	1471	1479	rBV	291171	386530	54.14%	10.983%
24	11.085	1634	1640	1646	rBV	370057	484489	67.86%	13.767%
25	12.024	1788	1794	1804	rBV	292885	363855	50.96%	10.339%

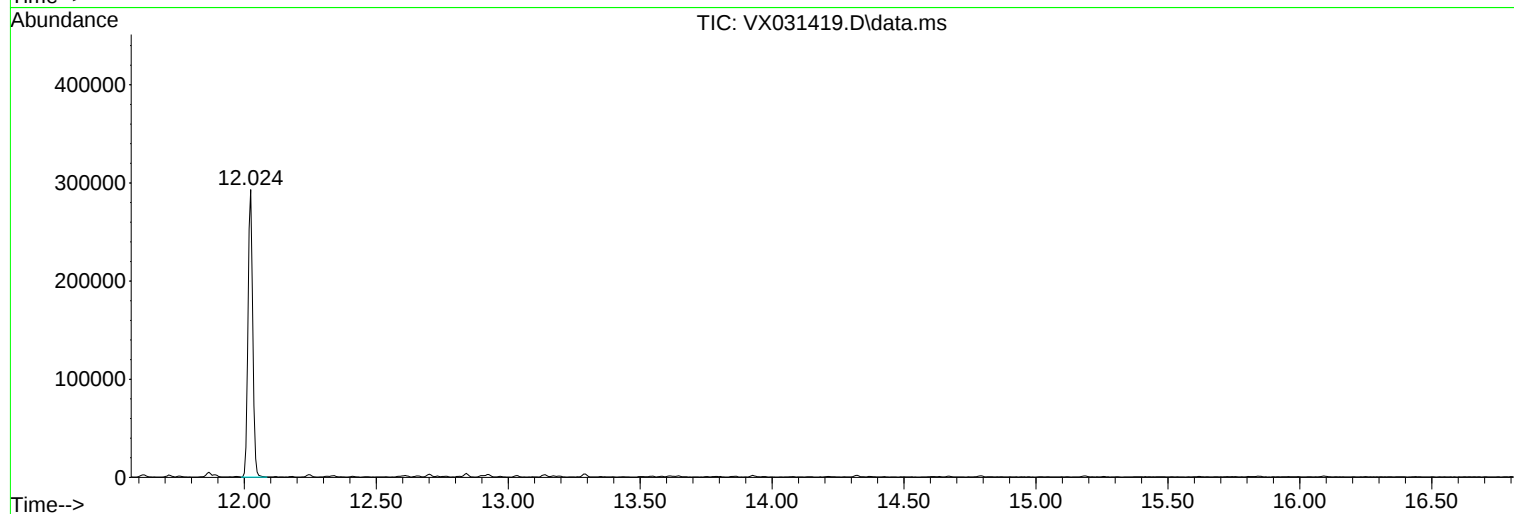
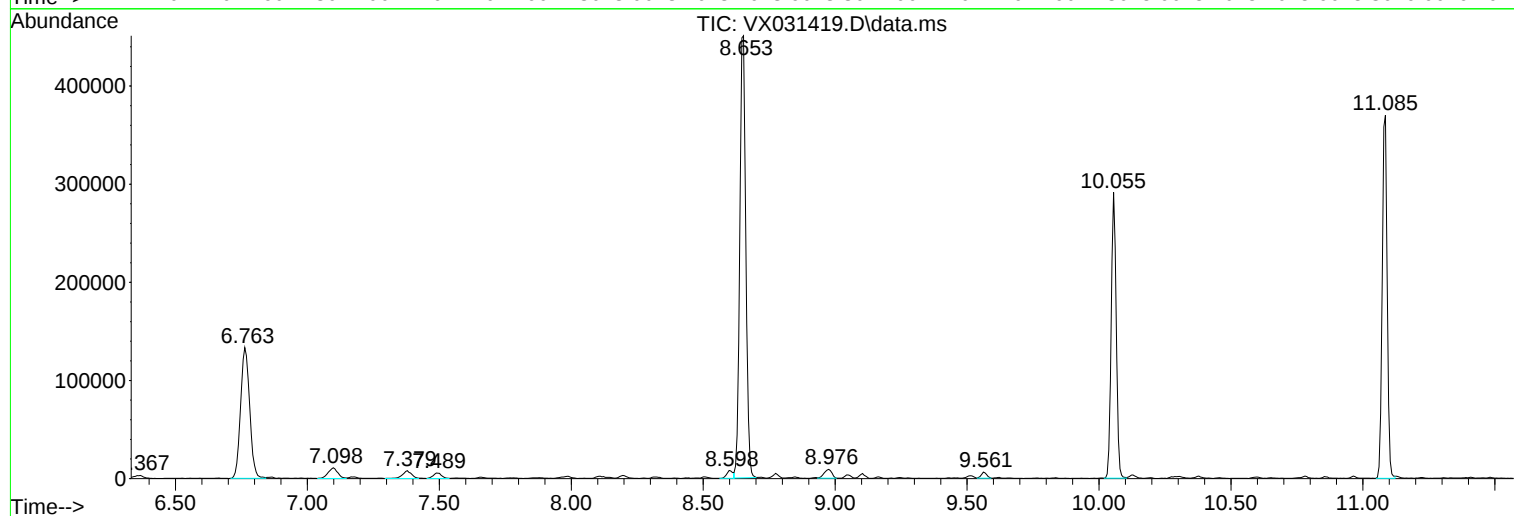
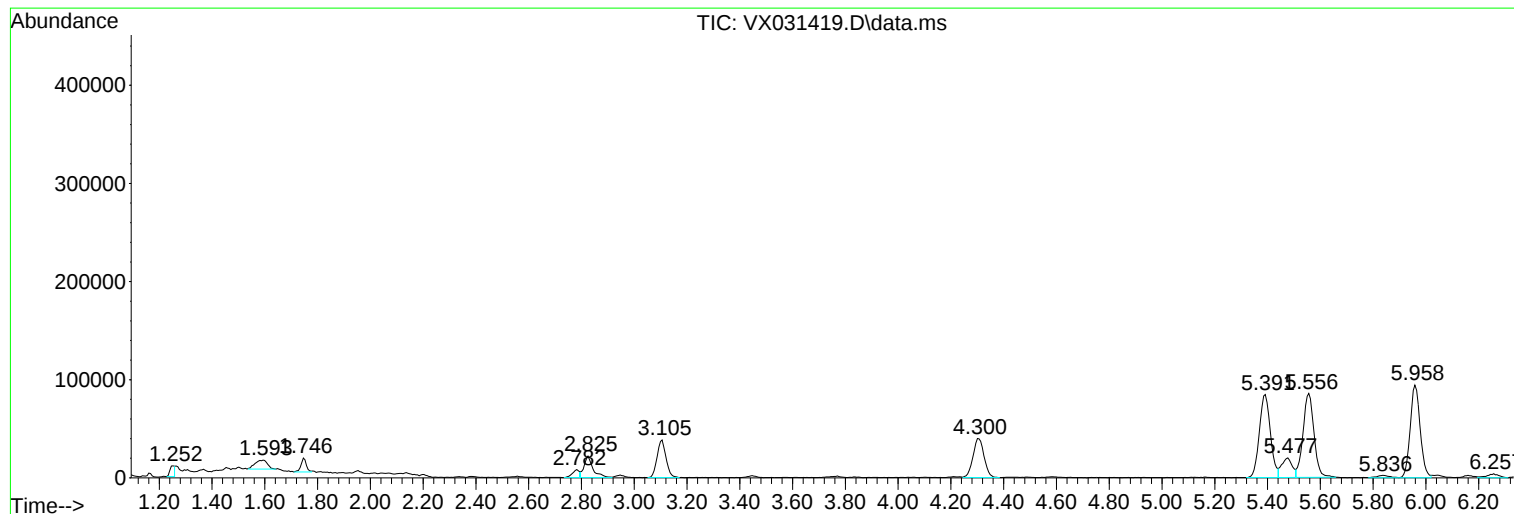
Sum of corrected areas: 3519255

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Instrument :
MSVOA_X
ClientSampleId :
TOLL-MW-02

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X091422W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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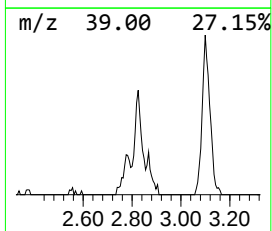
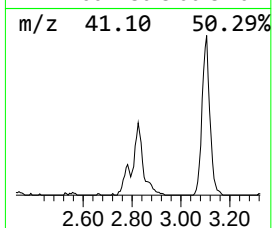
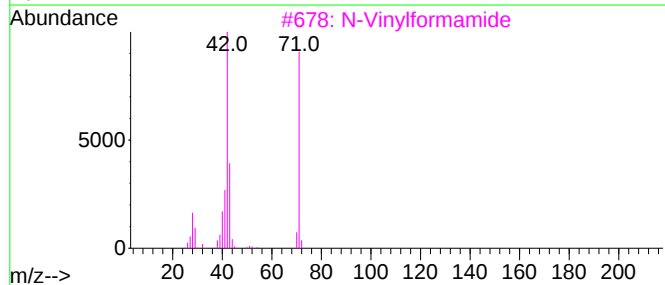
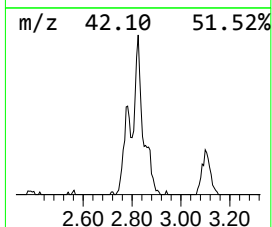
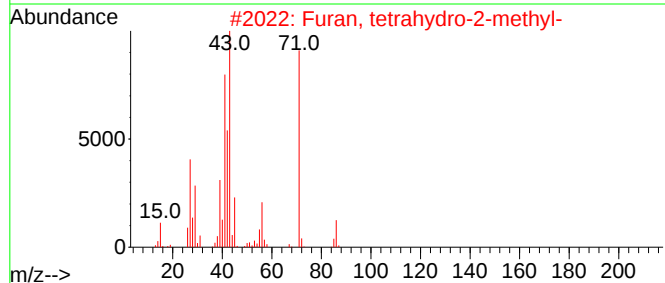
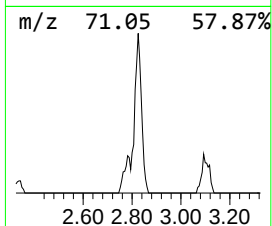
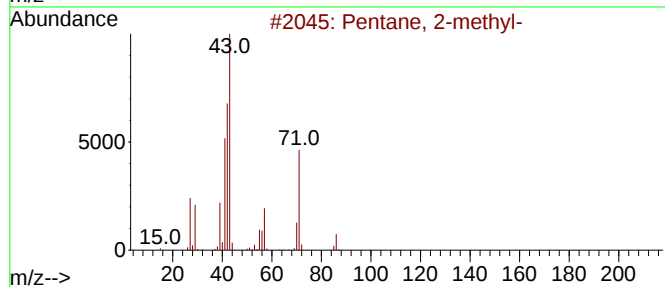
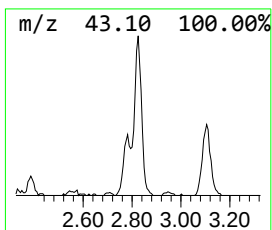
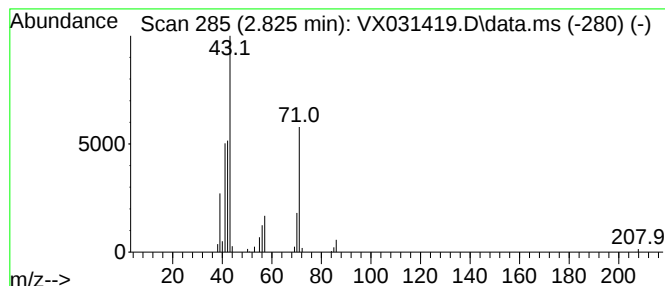
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X091422W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Pentane, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.825	10.20 ug/l	50251	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2-methyl-	86	C6H14	000107-83-5	83
2			Furan, tetrahydro-2-methyl-	86	C5H10O	000096-47-9	52
3			N-Vinylformamide	71	C3H5NO	013162-05-5	50
4			Pentane	72	C5H12	000109-66-0	38
5			Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	38



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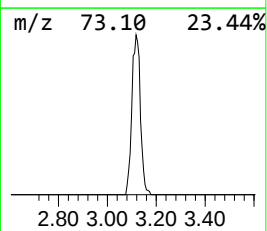
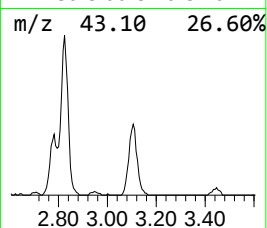
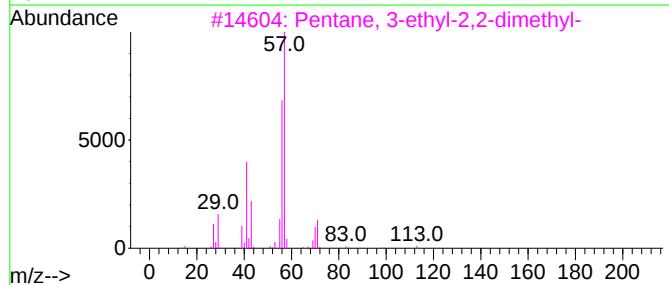
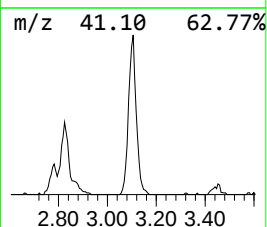
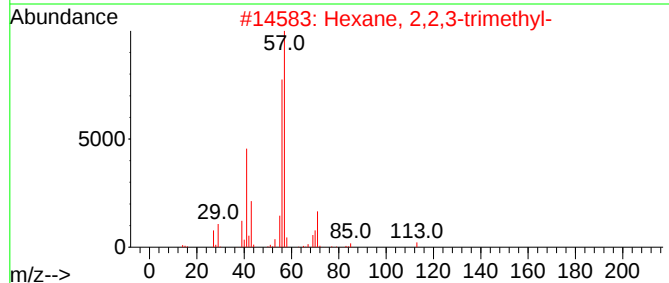
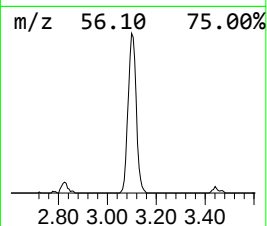
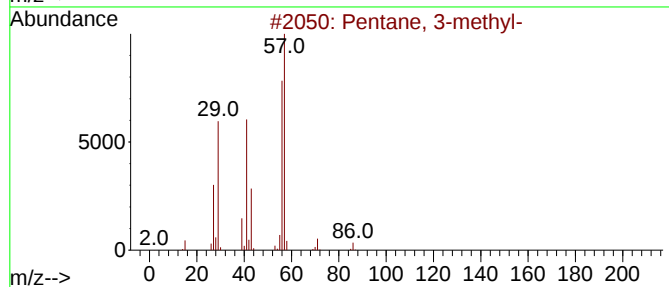
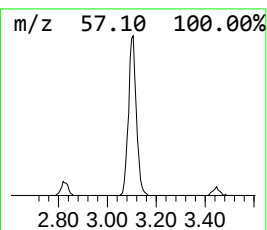
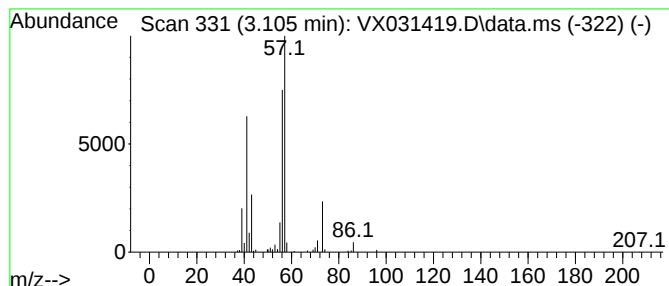
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TIC Integration Parameters: LSCINT.P

Peak Number 3 Pentane, 3-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.105	18.23 ug/l	89831	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 3-methyl-	86	C6H14	000096-14-0	83
2			Hexane, 2,2,3-trimethyl-	128	C9H20	016747-25-4	64
3			Pentane, 3-ethyl-2,2-dimethyl-	128	C9H20	016747-32-3	64
4			Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	40
5			Butyl isocyanatoacetate	157	C7H11NO3	017046-22-9	39



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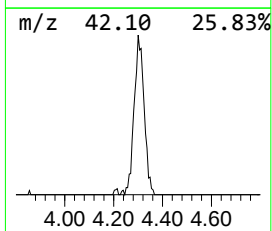
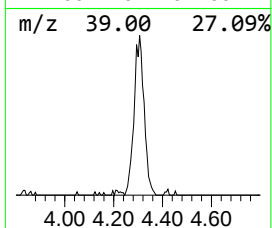
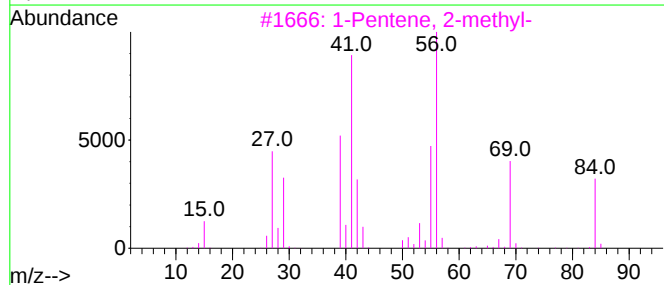
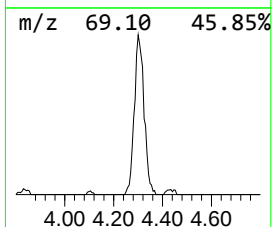
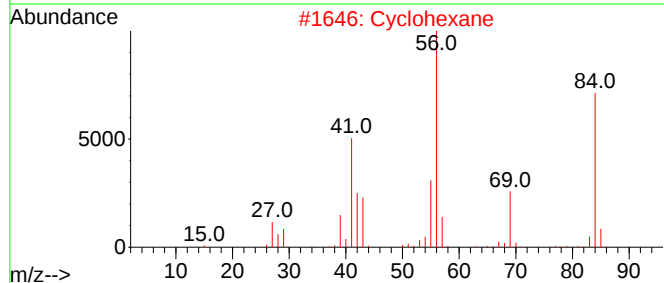
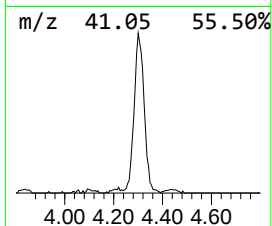
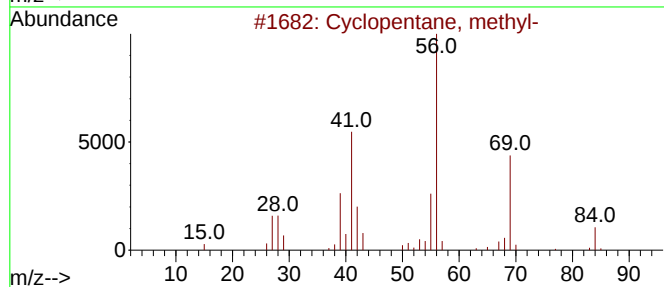
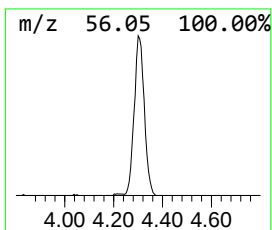
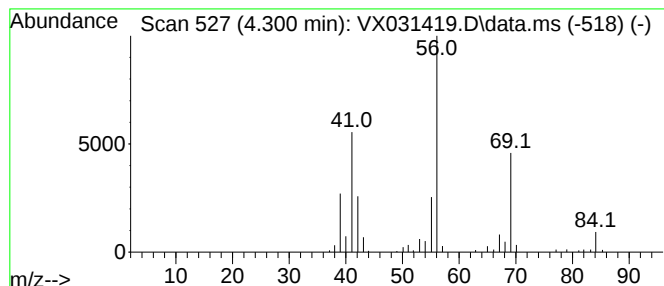
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TIC Integration Parameters: LSCINT.P

Peak Number 4 Cyclopentane, methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.300	23.45 ug/l	115572	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, methyl-	84	C6H12	000096-37-7	83
2			Cyclohexane	84	C6H12	000110-82-7	78
3			1-Pentene, 2-methyl-	84	C6H12	000763-29-1	43
4			1-Pentanol, 3-methyl-	102	C6H14O	000589-35-5	38
5			Cyclobutane, ethyl-	84	C6H12	004806-61-5	35



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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Pentane, 2-methyl-	2.825	10.2	ug/l	50251	1	5.556	246432	50.0
Pentane, 3-methyl-	3.105	18.2	ug/l	89831	1	5.556	246432	50.0
Cyclopentane, m...	4.300	23.4	ug/l	115572	1	5.556	246432	50.0